WHAT IS CLAIMED IS:

1. A system for analyzing mass spectrometric data comprising:

an data input means for entering mass spectrometric data of a parent ion and dissociated ions resulting from multiple dissociation of the parent ion; and

an analytical means for providing characteristics of a candidate for estimated structure of a precursor ion which is representative of pre-dissociation structure at each stage of dissociation,

wherein the system analyzes one of the structure of precursor ion at each stage of dissociation and the structure of parent ion based on the characteristics and spectrometric data.

2. A system according to claim 1 wherein the data input means receives data resulting from the multiple dissociation of the parent ion.

3. A system according to claim 2 further comprising:

a validity judging means for judging validity of candidates for the parent ion after dissociation of a precursor ion;

a displaying means for displaying the validity; and

a selection input means for entering selection for further dissolution.

4. A system according to claim 2 further comprising:

a validity judging means for judging validity of candidates for the parent ion after dissociation of a precursor ion,

wherein the system determines specifics for further dissociation according to the validity.

5. A system according to claim 1 wherein the analytical means provides a portion susceptible to separation for the candidate for the estimated structure of the precursor ion and the system has a displaying means for displaying the portion.

6. A system according to claim 1 wherein the analytical means provides the candidate for the estimated structure of the precursor ion with a value associated with strength of bonding between atoms and the system has a displaying means for displaying the value.

7. A system according to claim 1 wherein the analytical means provides a value associated with strength of bonding between atoms and the system displays the value.

8. A system according to claim 1 wherein the analytical means provides the candidate for the estimated structure of the precursor ion with a value associated with susceptibility to attachment for one of a proton and a positive ion, and the system has a displaying means for displaying the value.

9. A system according to claim 1 wherein the analytical means provides the candidate for the estimated structure of the precursor ion with a value associated with molecular orbit.

10. A system according to claim 9 wherein the value provided by the analytical means is related to one of a highest occupied molecular orbit, a lowest unoccupied molecular orbit, a first peripheral molecular orbit of the

highest occupied molecular orbit and a second peripheral molecular orbit of the lowest unoccupied molecular orbit, and the system has a displaying means for displaying the value.

11. A system according to claim 1 wherein the analytical means provides a value related to one of an electric charge distribution and an electrostatic potential for the candidate for the estimated structure of the precursor ion in a neutral condition, and the system displays the value.

12. A system according to claim 1 wherein the analytical means provides the characteristics of the candidate for the estimated structure of the precursor ion by introducing one of a molecular orbital calculation and a molecular dynamic calculation.

13. A system according to claim 1 further comprising a ranking means for providing ranking for the candidate for the estimated structure of the precursor ion based on the characteristics thereof obtained by the analytical means and the mass spectrometric data received by the data input means and wherein the system displays the ranking.

14. A system according to claim 1 further comprising a displaying means for displaying the characteristics of the candidate for the estimated structure of the precursor ion obtained by the analytical means, wherein the displaying means is adapted to display the characteristics utilizing one of distribution, colors, symbols and gradation.

15. A system according to claim 1 further comprising a structural search means for providing structure of a base attached to the precursor ion by modification, wherein the structural search means compares the characteristics of the candidate for the estimated structure of the precursor ion with the mass spectrometric data for the dissociated ions at each stage of dissociation, and wherein the system has a displaying means for displaying the structure of the base.

16. A system according to claim 15 wherein the displaying means is adapted to display both the estimated structure of the precursor ion and the structure of the base simultaneously.

17. A system according to claim 1, wherein the analytical means judges validity of the candidate for the estimated structure of the precursor ion, by comparing ionic strength of a dissociated ion having a peak value and measured ionic strength of the dissociated ion.

18. A system for analyzing structure of a compound comprising:

means for dissociating a parent ion;

means for entering mass spectrometric data for the parent ion and dissociated ions dissociated from the parent ion;

means for providing characteristics of a candidate for estimated structure of a precursor ion which is representative of pre-dissociation structure at each stage of dissociation,

wherein the system analyzes one of the structure of the precursor ion at each stage of dissociation and structure of the parent ion according to the

characteristics and mass spectrometric data.

19. A computer program for a computer of a system for analyzing mass spectrometric data, wherein the computer program executes the computer in a process comprising:

entering mass spectrometric data of a parent ion and dissociated ions resulting from multiple dissociation of the parent ion in an data input means; and

providing characteristics of a candidate for estimated structure of a precursor ion which is representative of pre-dissociation structure at each stage of dissociation,

wherein the computer program executes the computer to analyze one of the structure of precursor ion at each stage of dissociation and the structure of parent ion based on the characteristics and spectrometric data.